

## Index of Authors

with the titles of papers

- ADYA, A. K., and NELSON, G. W.: The structure of molten ammonium nitrate by isotopic difference method of neutron diffraction, 747
- ALAVI, A., and McDONALD, I. R.: Molecular-dynamics simulation of argon physisorbed on magnesium oxide, 703
- ANGLADA, J., BRUNA, P. J., and PEYERIMHOFF, S. D.: Theoretical investigation of the low-lying electronic states of TiH, 281
- BALASUBRAMANIAN, K., *see* Wang, J. Z.
- BALFOUR, W. J., LAUNILA, O., and KLYNNING, L.: Fourier transform spectroscopy of MnH and MnD. Rotational analyses of the 846 nm and 1060 nm systems, 443
- BARNICKEL, P., and WOKAUN, A.: Synthesis of metal colloids in inverse microemulsions, 1
- BECKMANN, P. A., HATHORN, R. M., and MALLORY, F. B.: Proton Zeeman relaxation and intramolecular reorientation in solid *t*-butylbenzene, 411
- BEDANOV, V. M.: Computer simulation of cluster decay, 1011
- BELL, A. J., and FREY, J. G.: Raman emission from the photolysis of NOCl at 266 nm, 943
- BERG, L.-E., ROYEN, P., and WEUNITZ, P.: Lifetime measurements of CaCl, CaBr and SrCl. Radiative lifetimes of the  $B^2\Sigma^+$  states, 385
- BERMEJO, F. J., *see* Esteban, A. L.
- BISWAS, S. N., *see* Sun, T. F.
- BODEN, N., *see* Kahol, P. K.
- BOUBLIK, T.: Perturbation theory of pure quadrupolar hard gaussian overlap fluids, 497
- BROUARD, M., MARTINEZ, M. T., O'MAHONY, J., and SIMONS, J. P.: Energy and angular momentum disposals in the vibrationally mediated photodissociation of HOOH and HOOD. Intramolecular properties via photofragment mapping, 65
- BROWN, J. M., *see* Steimle, T. C.
- BROWN, M. F., SALMON, A., HENRIKSSON, U., and SÖDERMAN, O.: Frequency dependent  $^2\text{H}$  N.M.R. relaxation rates of small unilamellar phospholipid vesicles, 379
- BRUNA, P. J., *see* Anglada, J.
- BURNELL, E. E., *see* Zimmerman, D. S.
- CAILLOL, J. M., LEVESQUE, D., and WEIS, J. J.: Monte Carlo simulation of an ion-dipole mixture. A convergence study, 199
- CARLEER, M., *see* Ndikumana, T.
- COLIN, R., *see* Ndikumana, T.
- CZUMAJ, Z.: Absorption coefficient and refractive index measurements of water in the millimetre spectral range, 787
- DAS, K. K., *see* Wang, J. Z.
- DAVIDENKO, N. A., *see* Kuvshinsky, N. G.
- DAVIES, P. B., and DAVIS, I. H.: Far infrared L.M.R. of  $\tilde{X}^2\Pi$  NCO, 175
- DAVIS, I. H., *see* Davies, P. B.
- DE ALMEIDA, W. B., and HINCHLIFFE, A.: *Ab initio* vibrational spectrum of the H-bonded trimers (HCN)<sub>2</sub>HF and HCN(HF)<sub>2</sub>, 305

- DE HAAG, P. U., SPOOREN, R., EBBEN, M., MEERTS, L., and HOUGEN, J. T.: Internal rotation in 1,4-dimethylnaphthalene studied by high resolution laser spectroscopy, 265
- DELFS, C. D., and FIGGIS, B. N.: Magnetization density in *trans*-tetraamminedinitronickel(II), 401
- DE SANTIS, A., and GREGORI, A.: Induced contributions in the Rayleigh band of gaseous  $\text{H}_2\text{O}$ , 715
- DIEZ, E., *see* Esteban, A. L.
- DOWNS, D. W., *see* Yenice, K. M.
- EBBEN, M., *see* de Haag, P. U.
- EDWARDS, P. P., ELLABOUDY, A. S., HOLTEN, D. M., and PYPER, N. C.: The chemical dynamics of  $\text{Na}^+$  in liquid 12-crown-4 solutions deduced from  $^{23}\text{Na}$  nuclear spin relaxation rates, 209
- ELLABOUDY, A. S., *see* Edwards, P. P.
- ENGELS, B., *see* Karna, S. P.
- ESTEBAN, A. L., GALACHE, M. P., DIEZ, E., SAN FABIAN, J., and BERMEJO, F. J.: Dependence of the dipolar couplings of tetrahydrofuran on the pseudorotation parameters, 429
- EVANS, D. J., *see* Murad, S.
- EVANS, M. W., and HEYES, D. M.: Combined shear and elongational flow by non-equilibrium molecular dynamics, 241
- FARANTOS, S. C., *see* Vegiri, A.
- FIGGIS, B. N., *see* Delfs, C. D.
- FISCHER, J., *see* Möller, D.
- FLETCHER, D. A., *see* Steimle, T. C.
- FOSTER, S. C., *see* Liu, X.
- FRANK, U. E., HERDEG, W., GHOSH, P. N., and HÜTTNER, W.: MW and mm wave spectra, octic-order centrifugal-distortion,  $^{14}\text{N}$  nuclear electric quadrupole coupling, and dipole moment of the gauche tetrafluorohydrazine conformer,  $\text{N}_2\text{F}_4$ , 33
- FREY, J. G., *see* Bell, A. J.
- FREY, J. G., and HOLDSHIP, S. J.: Calculation of non-adiabatic matrix elements, 783
- FURER, N., *see* Stranger, R.
- GALACHE, M. P., *see* Esteban, A. L.
- GHOSH, P. N., *see* Frank, U. E.
- GIRARD, C., *see* Labani, B.
- GOCHIN, M., PINES, A., ROSEN, M. E., RUCKER, S. P., and SCHMIDT, C.: Two-dimensional N.M.R. studies of flexible molecules in liquid crystals: orientational order and conformational probabilities of *n*-hexane, 671
- GRAY, C. G., *see* Joslin, C. G.
- GREGORI, A., *see* De Santis, A.
- GREIN, F., *see* Karna, S. P.
- GRUEBELE, M.: Numerical potential functions for diatomic molecules. The *f*-potentials of  $\text{CF}^+$  and  $\text{CCl}^+$ , 475
- GÜDEL, H., *see* Stranger, R.
- HABASAKI, J.: Molecular dynamics simulation of molten  $\text{Li}_2\text{CO}_3$  and  $\text{Na}_2\text{CO}_3$ , 115
- HANLEY, H. J. M., *see* Wielopolski, P. A.
- HARRISON, K. J., *see* McEwan, K. J.
- HATHORN, R. M., *see* Beckmann, P. A.
- HENDERSON, J. R., and TENNYSON, J.: Very highly excited vibrational states of LiCN using a discrete variable representation, 639
- HENRIKSSON, U., *see* Brown, M. F.
- HERDEG, W., *see* Frank, U. E.

- HERNANDO, J. A.: Thermodynamic potentials and distribution functions. I. A general expression for the entropy, 319
- HERNANDO, J. A.: Thermodynamic potentials and distribution functions. II. The HNC equation as an optimized superposition approximation, 327
- HEYES, D. M.: Cluster analysis and continuum percolation of 3D square-well phases. MC and PY solutions, 559
- HEYES, D. M., *see* Evans, M. W.
- HINCHLIFFE, A., *see* De Almeida, W. B.
- HOHM, U., and KERL, K.: Interferometric measurements of the dipole polarizability  $\alpha$  of molecules between 300 K and 1100 K. I. Monochromatic measurements at  $\lambda = 632.99$  nm for the noble gases and  $H_2$ ,  $N_2$ ,  $O_2$ , and  $CH_4$ , 803
- HOHM, U., and KERL, K.: Interferometric measurements of the dipole polarizability  $\alpha$  of molecules between 300 K and 1100 K. II. A new method for measuring the dispersion of the polarizability and its application to Ar,  $H_2$ , and  $O_2$ , 819
- HOLDSHIP, S. J., *see* Frey, J. G.
- HOLTON, D. M., *see* Edwards, P. P.
- HOŁYST, R., and PONIEWIERSKI, A.: Study of the Landau bicritical point in dense systems of hard biaxial molecules, 193
- HOUGEN, J. T., *see* de Haag, P. U.
- HOWARD, B. J., *see* Randall, R. W.
- HOWE, M. A.: Orientational correlations in the liquid halogens, 161
- HÜTTNER, W., *see* Frank, U. E.
- IGLESIAS-SILVA, G. A., *see* Nezbeda, I.
- JANSSEN, R., *see* van der Mijden, J. A. M.
- JOSLIN, C. G., GRAY, C. G., MICHELS, J. P. J., and KARKHECK, J.: The bulk viscosity of a square-well fluid, 535
- KAHOL, P. K., and BODEN, N.: N.M.R. solid echoes in systems of dipolar-coupled inequivalent spins-1 or dipolar-coupled inequivalent pairs of spins-1/2, 833
- KARKHECK, J., *see* Joslin, C. G.
- KARNA, S. P., and GREIN, F.: *Ab initio* SCF and CI studies of the electric field gradient in LiH, 661
- KARNA, S. P., GREIN, F., ENGELS, B., and PEYERIMHOFF, S. D.: *Ab initio* configuration-interaction studies of the ground state potential energy and hyperfine coupling constants of  $^{35}Cl_2^-$ , 549
- KERL, K., *see* Hohm, U.
- KLYNNING, L., *see* Balfour, W. J.
- KORTBEEK, P. J., and SCHOUTEN, J. A.: Calculation of thermodynamic properties of dense fluid neon using statistical-mechanical perturbation theory. Part I: Method, potentials and results up to 1 GPa, 981
- KORTBEEK, P. J., *see* Sun, T. F.
- KORTBEEK, P. J., TEN SELDAM, C. A., and SCHOUTEN, J. A.: Calculation of thermodynamic properties of dense fluid neon using statistical-mechanical perturbation theory. Part II: Results up to 6 GPa and equations of state, 1001
- KRAUSZ, E., *see* Stranger, R.
- KUVSHINSKY, N. G., DAVIDENKO, N. A., and RESHETNYAK, V. V.: On the influence of electron localization radius in a charge-transfer complex on photogeneration efficiency of current carriers in carbazole-containing semiconductors, 933
- LABANI, B., GIRARD, C., and MAGHEZZI, S.: van der Waals interactions between a molecule and a small metallic sphere, 85
- LABÍK, S., SMITH, W. R., POSPÍŠIL, R., and MALUEVSKÝ, A.: Non-spherical bridge function theory of molecular fluids. I. The hard-dumbbell fluid, 649

- LAUNILA, O., *see* Balfour, W. J.  
LEE, S. A., *see* Yenice, K. M.  
LEVANT, D., *see* Moreh, R.  
LEVESQUE, D., *see* Caillol, J. M.  
LIU, X., FOSTER, S. C., WILLIAMSON, J. M., YU, L., and MILLER, T. A.: The spin-rotation interactions in the methoxy radical, 357
- MCDONALD, I. R., *see* Alavi, A.  
MCEWAN, K. J., HARRISON, K. J., and MADDEN, P. A.: Polarisation and material dependence of degenerate four-wave mixing transients in molecular fluids, 1025  
MADDEN, P. A., *see* McEwan, K. J.  
MAGHEZZI, S., *see* Labani, B.  
MAKAREWICZ, J.: Semiclassical and quantum mechanical pictures of the ro-vibrational motion of triatomic molecules, 903  
MALESCIO, G.: Excess electrons in molten salts. Polaron theory of dilute Cs-CsI solutions, 895  
MALJEVSKÝ, A., *see* Labík, S.  
MALLORY, F. B., *see* Beckmann, P. A.  
MAN, P. P.: Measurement of quadrupolar coupling with a two-pulse sequence in solid-state N.M.R., 337  
MARTINEZ, M. T., *see* Brouard, M.  
MARUANI, J., *see* Mezey, P. G.  
MEERTS, L., *see* de Haag, P. U.  
MERCER, J. M.: Effective isotropic dipole-dipole pair potential, 625  
MESTECHKIN, M. M., and WHYMAN, G. E.: Structural influence on ferromagnetic ordering in quasi-one-dimensional systems, 775  
MEZEY, P. G., and MARUANI, J.: The concept of 'syntopy'. A continuous extension of the symmetry concept for quasi-symmetric structures using fuzzy-set theory, 97  
MICHELS, J. P. J., *see* Joslin, C. G.  
MILLER, T. A., *see* Liu, X.  
MÖLLER, D., and FISCHER, J.: Vapour liquid equilibrium of a pure fluid from test particle method in combination with  $NpT$  molecular dynamics simulations, 463  
MONTONE, A., and SACCHETTI, F.: Structure of the amorphous phase of sodium hydroxide, 1073  
MORAN, G., *see* Stranger, R.  
MOREH, R., and LEVANT, D.: NRPS study of nitric oxide adsorption on activated carbon fibre, 735  
MOTTRAM, R. E., *see* Murrell, J. N.  
MUENTER, J. S., *see* Randall, R. W.  
MURAD, S., and EVANS, D. J.: Heat induced polarization in molecular fluids, 697  
MURRELL, J. N., and MOTTRAM, R. E.: Potential energy functions for atomic solids, 571
- NACHMAN, D. F., *see* Steimle, T. C.  
NDIKUMANA, T., CARLEER, M., and COLIN, R.: Laser-induced fluorescence spectrum and radiative lifetimes of the gaseous PbSe molecule, 229  
NEILSON, G. W., *see* Adya, A. K.  
NEZBEDA, I., and IGLESIAS-SILVA, G. A.: Primitive model of water. III. Analytic theoretical results with anomalies for the thermodynamic properties, 767
- OGINO, Y., *see* Yamazaki, T.  
O'MAHONY, J., *see* Brouard, M.  
OZAWA, S., *see* Yamazaki, T.
- PACKER, M. J., and RAYNES, W. T.: Electric field effects on the  $^{13}\text{C}$  and  $^{19}\text{F}$  nuclear shielding in HF and  $\text{CH}_3\text{F}$ , 391  
PERCUS, J. K., and ZHANG, M. Q.: The quasi-one dimensional hard square gas, 347

- PEYERIMHOFF, S. D., *see* Anglada, J.  
PEYERIMHOFF, S. D., *see* Karna, S. P.  
PINES, A., *see* Gochin, M.  
PONIEWIERSKI, A., *see* Holyst, R.  
POSPISIL, R., *see* Labik, S.  
PRICE, S. L., *see* Wheatley, R. J.  
PYPER, N. C., *see* Edwards, P. P.
- QUACK, M., and SUHM, M. A.: Potential energy surface and energy levels of (HF)<sub>2</sub> and its D isotopomers, 791
- RANDALL, R. W., WILKIE, J. M., HOWARD, B. J., and MUENTER, J. S.: Infrared vibration-rotation spectrum and structure of OCS dimer, 839  
RAYNES, W. T., *see* Packer, M. J.  
RESHETNYAK, V. V., *see* Kuvshinsky, N. G.  
REYNHARDT, E. C.: An NMR, DSC and X-ray investigation of the disaccharides sucrose, maltose and lactose, 1083  
RITTGER, E.: The chemical potential of liquid xenon by computer simulation, 853  
RITTGER, E.: Can three-atom potentials be determined from thermodynamic data?, 867  
ROSEN, M. E., *see* Gochin, M.  
ROYEN, P., *see* Berg, L.-E.  
RUCKER, S. P., *see* Gochin, M.
- SACCHETTI, F., *see* Montone, A.  
SALMON, A., *see* Brown, M. F.  
SAN FABIAN, J., *see* Esteban, A. L.  
SCHMIDT, C., *see* Gochin, M.  
SCHOUTEN, J. A., *see* Kortbeek, P. J.  
SCHOUTEN, J. A., *see* Sun, T. F.  
SHIRLEY, J. E., *see* Steimle, T. C.  
SIMONS, J. P., *see* Brouard, M.  
SINHA, S. K.: Semiclassical statistical mechanics of a  $\nu$ -dimensional fluid of hard  $\nu$ -spheres. I. Equilibrium properties of dilute hard  $\nu$ -sphere gas, 587  
SMITH, W. R., *see* Labik, S.  
SÖDERMAN, O., *see* Brown, M. F.  
SPOOREN, R., *see* de Haag, P. U.  
STEIMLE, T. C., NACHMAN, D. F., SHIRLEY, J. E., FLETCHER, D. A., and BROWN, J. M.: The microwave spectrum of NiH, 923  
STRANGER, R., MORAN, G., KRAUSZ, E., GÜDEL, H., and FÜRER, N.: Octahedral monomeric molybdenum(III). A magneto-optical study of Mo<sup>3+</sup> doped in Cs<sub>2</sub>NaYCl<sub>6</sub>, 11  
SUHM, M. A., *see* Quack, M.  
SUN, T. F., and SCHOUTEN, J. A.: The importance of accurate numerical integration in perturbation theories of molecular liquids, 601  
SUN, T. F., SCHOUTEN, J. A., TEN SELDAM, C. A., and BISWAS, S. N.: Perturbation calculation of thermodynamic properties of liquid benzene using the six centre Lennard-Jones potential, 615  
SUN, T. F., SCHOUTEN, J. A., TEN SELDAM, C. A., and KORTBEEK, P. J.: An efficient algorithm for the solution of the correlation function for soft spherical repulsions, 607
- TEN SELDAM, C. A., *see* Kortbeek, P. J.  
TEN SELDAM, C. A., *see* Sun, T. F.  
TENNYSON, J., *see* Henderson, J. R.  
TOMASELLO, P., and VON NIESSEN, W.: Electronic structure of lithium halide monomers and dimers: ionization energies and electron affinities, 1043

- VAN DER MIJDE, J. A. M., JANSSEN, R., and VEEMAN, W. S.: Analytical description of the  $I = \frac{5}{2}$  quadrupole nutation experiment, 53
- VEEMAN, W. S., *see* van der Mijde, J. A. M.
- VEGIRI, A., and FARANTOS, S. C.: A classical dynamical investigation of the mechanism of electronic quenching of  $\text{OH}(A^2\Sigma^+)$  in collisions with  $\text{CO}(X^1\Sigma^+)$ , 129
- VON NIESSEN, W., *see* Tomasello, P.
- WANG, J. Z., DAS, K. K., and BALASUBRAMANIAN, K.: Potential energy surfaces for insertion of Zr into  $\text{H}_2$ , 147
- WEINIZ, P., *see* Berg, L.-E.
- WEIS, J. J., *see* Caillol, J. M.
- WHEATLEY, R. J., and PRICE, S. L.: An overlap model for estimating the anisotropy of repulsion, 507
- WHITE, J. W., *see* Wielopolski, P. A.
- WHYMAN, G. E., *see* Mestechkin, M. M.
- WIELOPOLSKI, P. A., and WHITE, J. W.: Dynamics of the intercalated layer in  $\text{C}_{36}\text{Cs}$ : dependence on the temperature and substrate potential, 959
- WIELOPOLSKI, P. A., WHITE, J. W., and HANLEY, H. J. M.: Structure of a stage-3 Cs-graphite intercalate, 947
- WILKIE, J. M., *see* Randall, R. W.
- WILLIAMSON, J. M., *see* Liu, X.
- WOKAUN, A., *see* Barnickel, P.
- YAMAZAKI, T., OZAWA, S., and OGINO, Y.: Potential energies for methane adsorption in ion-exchanged ZSM-5 zeolite pore, 369
- YENICE, K. M., LEE, S. A., and DOWNS, D. W.: Optical properties of methanol at high pressures, 973
- YU, J., *see* Liu, X.
- ZHANG, M. Q., *see* Percus, J. K.
- ZIMMERMAN, D. S., and BURNELL, E. E.: Size and shape effects on the orientation of solutes in nematic liquid crystals, 1059

